Rise and fall of hidden string order of lattice bosons

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We investigate the ground state properties of a newly discovered phase of one dimensional lattice bosons with extended interactions[6]. The new phase, termed the Haldane Insulator (HI) in analogy with the gapped phase of spin-1 chains, is characterized by a non local order parameter, which can only be written as an infinite string in terms of the bosonic densities. We show that the string order can nevertheless be probed with physical fields that couple locally, via the effect those fields have on the quantum phase transitions separating the exotic phase from the conventional Mott and density wave phases. Using a field theoretical analysis we show that a perturbation which breaks lattice inversion symmetry gaps the critical point separating the Mott and Haldane phases and eliminates the sharp distinction between them. This is remarkable given that neither of these phases involves broken inversion symmetry. We also investigate the evolution of the phase diagram with the tunable coupling between parallel chains in an optical lattice setup. We find that inter-chain tunneling destroys the direct phase transition between the Mott and Haldane insulators by establishing an intermediate superfluid phase. On the other hand coupling the chains only by weak repulsive interactions does not modify the structure of the phase diagram. The theoretical predictions are confirmed with numerical calculations using the Density Matrix Renormalization Group (DMRG).

I. INTRODUCTION

Systems of ultracold bosons in optical lattices offer unique opportunities for studying strongly correlated quantum matter in a highly controllable environment[1]. In a sufficiently deep lattice potential the interactions dominate over the kinetic energy and, at commensurate filling, can drive a quantum phase transition from the superfluid to the Mott insulating state. This transition has been observed experimentally[2], and it requires only local (on-site) interactions between the bosons. Longer range interactions, effective for example in systems of ultracold polar molecules[3] or atoms with large magnetic dipole moment[4,5] , can give rise to even richer behavior. In particular, we have recently predicted that bosons with sufficiently strong nearest neighbor or further range repulsion on a one dimensional lattice form a new insulating ground state characterized by hidden topological order[6].

We termed the new phase a Haldane Insulator (HI) because of the close analogy with Haldane's gapped phase of integer spin-chains[7]. Both states support a highly non local string order parameter[8,9,10]. Moreover, the phase transitions from the Haldane insulating phase to the conventional Mott and Density wave (DW) insulators, also have their analogies in anisotropic spin chains[8,12,13]. This phase can potentially be realized in a system of cold dipolar atoms or molecules in a one dimensional optical lattice, where the dipole moment is polarized perpendicular to the chain direction.

There are, however, essential differences between the spin chains and the lattice bosons. First, the anisotropic spin chains enjoy a global Z_2 symmetry associated with flipping the S^z component of all spins. This would translate to a particle-hole symmetry about the mean lattice filling, which is clearly absent in the microscopic bosonic models. Furthermore, the optical lattice systems are in practice not strictly one dimensional. Some amount of residual coupling between chains due to tunneling and, in our case, also dipolar interactions, is inevitable. More generally, we shall see that additional external fields, which can be applied to the ultracold Bose systems, couple in a non trivial way to the string order parameter. The effects of these perturbations on the phase diagram raise new fundamental questions on the nature of the non local order.

In this paper we investigate how different perturbations, natural to bosonic systems, affect the transitions from the Haldane insulator to the conventional Mott and Density wave phases. We argue that these directly probe the nature of the non local order parameter which characterizes the Haldane insulator phase. Using a bosonization analysis, we demonstrate that the transitions between the HI and the conventional phases are not sensitive to the broken particle-hole symmetry in the microscopic Hamiltonian. Such perturbations also leave the string order parameter intact. On the other hand we predict that perturbations that break the lattice inversion symmetry in addition to the particle-hole symmetry, would eliminate the distinction between the MI and HI phases and gap out the critical point separating them. Next we investigate the effect of coupling between two parallel chains ("ladder" geometry). The predictions of the field theoretical analysis are confirmed with numerical simulations using the Density Matrix Renormalization Group (DMRG) method.

Our starting point for theoretical analysis is the extended Bose Hubbard model (EBHM) on one or two

FIG. 1: (Color online.) Array of one dimensional chains formed by a two dimensional optical lattice. The polarizing field E is directed perpendicular to the chains and at an angle θ which can be used to tune the inter-chain interaction $V_\perp$ in (2).

chains at single site occupation ($\bar{n} = 1$):

$$H_\alpha = -t \sum_j \left(b^\dagger_{\alpha j} b_{\alpha j+1} + h.c. \right) + \frac{U}{2} \sum_j n_{\alpha j} \left(n_{\alpha j} - 1 \right) + V \sum_j n_{\alpha j} n_{\alpha j+1}, \quad (1)$$

where j is the site index and $\alpha = 1, 2$ is the chain index, in the case of two chains. The inter-chain coupling in that case includes a transverse tunneling matrix element and interaction term:

$$H_\perp = -t_\perp \sum_j (b^\dagger_{1j} b_{2j} + H.c.) + V_\perp \sum_j n_{1j} n_{2j}. \quad (2)$$

In practice the inter-chain tunneling $t_\perp$ may be tuned by varying the depth of the optical lattice potential in the direction perpendicular to the chains. The inter-chain dipolar interaction can be controlled by changing the direction of the external polarizing field relative to the plane of the chains, while keeping it perpendicular to the chain axis. A schematic setup of this type involving many coupled chains is illustrated in Fig. 1. The two chain model

$$H = \sum_{\alpha=1,2} H_\alpha + H_\perp \quad (3)$$

serves as a bridge between one and two dimensional geometries, while still amenable to powerful techniques for treating one dimensional systems, such as bosonization and the density matrix renormalization group (DMRG). Similar quasi one-dimensional systems were studied previously in different parameter regimes: with only on-site interactions[14,15] and with longer-range interactions at half-integer filling[16]. However, the Haldane insulator phase which is the focus of this paper is not obtained in these regimes.

Recently Anfuso and Rosch noted that the string order characterizing the Haldane gapped phase of spin-1 chains is unstable against inter-chain antiferromagnetic exchange[18]. The string order in the HI phase is similarly sensitive to inter-chain tunnel coupling (see appendix A), and the distinction between the HI and MI phases is lost. What is then the fate of the direct second order transition found between these two phases when inter-chain tunneling is turned on? Interestingly we find that direct transition between these two phases is avoided in the double chain system by the appearance of an intermediate superfluid phase for arbitrarily small inter-chain tunneling.

Our analysis consists of the following parts. In section II A we present a low energy effective field theory for the single chain, which correctly captures all three insulating phases MI, HI and DW. This is done with help of a special bosonization procedure borrowed from work on integer spin chains[12]. The bosonized forms for the non local correlations that characterize the HI and MI phases are given in section II B. This framework is used in section II C to study the coupling of the non local order parameters to inversion symmetry breaking perturbations. Then in section II D we extend the bosonization approach to describe a pair of weakly coupled chains. We carry out a renormalization group (RG) analysis to obtain analytic predictions for the phases arising at weak inter-chain coupling in the vicinity of the quantum critical points. The most interesting result of the coupling is the effect of inter-chain tunneling on the transition between the MI and HI states. This perturbation is highly relevant at the critical point. As a result we find that for any finite $t_\perp$ the HI and MI insulating phases are separated by a superfluid region, whose domain grows rapidly with increasing $t_\perp$. Finally in section III we confirm the analytic predictions and extend them to stronger inter-chain coupling using numerical DMRG calculations.

The paper is followed by three appendices. In appendix A we investigate the effect of weak inter-chain coupling deep in the HI phase within perturbation theory. Although the thermodynamic HI phase is protected by a gap Δ, we show that the single chain string order is destroyed even by infinitesimal coupling. In appendix B we provide an alternative derivation of the effective field theory using direct bosonization of the particles rather than resorting to an effective spin-1 model as done in section II. In appendix C we construct explicit expressions for the string order parameter within the effective field theory.

II. BOSONIZATION

A. Continuum limit of a single unperturbed chain

A single chain of interacting bosons (1) at filling $\bar{n} = 1$ was studied in Ref. [6] using DMRG and the existence of the new Haldane insulator (HI) phase was predicted. The phase diagram in the two dimensional space of U/t versus V/t is reproduced here in Fig. 4(a).

The insulating phases and the correct quantum phase transitions separating them can also be obtained from a field theoretical analysis[19], which builds on a direct analogy with the bosonization procedure developed for integer spin chains[11,12,20]. Let us briefly review the derivation of the effective field theory of a single chain. The

first step is an approximate mapping of the EBHM (1) to an anisotropic spin-1 model. This is done by truncation of the Hilbert space of each site to the three lowest occupation states $n = 0, 1, 2$[21,22]. Such a truncation is justified at large U when fluctuations in the site occupations are strongly suppressed. The effective spin-1 model is

$$H = -t\sum_j \left(S_j^+ S_{j+1}^- + h.c.\right) + \frac{U}{2}\sum_j \left(S_j^z\right)^2 + V\sum_j S_j^z S_{j+1}^z \tag{4}$$

Here $S^z = n - \bar{n}$. In general, there are other terms in this Hamiltonian which break the $S^z \to -S^z$, $S^+ \longleftrightarrow S^-$ ("particle-hole") symmetry. However, in the effective long-wavelength Hamiltonian we will now derive, these terms are irrelevant, so we will drop them for now. The effect of these terms will be considered in section II C.

One then proceeds by writing each spin 1 variable as a sum of two spin $\frac{1}{2}$ variables[11,12], $S_j^z = s_{1,j}^z + s_{2,j}^z$. Each spin-$\frac{1}{2}$ chain can now be mapped to a spinless fermion chain by a Jordan-Wigner transformation. The fermions are then bosonized in the standard way[17], according to $\psi_{\alpha,R/L} \sim \frac{1}{\sqrt{2\pi a}} e^{i(\theta_\alpha \pm \phi_\alpha)}$, where a is the lattice spacing, $\alpha = 1, 2$ corresponds to the two fictitious spin-1/2 chains (not to be confused with the two physical chains that will be considered in section II D) and R/L corresponds to right and left moving fermions, respectively. The bosonic fields satisfy the canonical commutation relations $[\phi_\alpha(x), \theta_\beta(x')] = -i\pi\delta_{\alpha,\beta}\Theta(x'-x)$, where $\Theta(x)$ is a Heaviside step function. With these conventions[23], the spin-1/2 operators have the following bosonized form:

$$s_\alpha^z = \frac{a}{\pi}\partial_x\phi_\alpha + \frac{(-1)^{\frac{x}{a}}}{\pi}\sin(2\phi_\alpha). \tag{5}$$

The bosonized Hamiltonian is conveniently written in terms of symmetric (+) and antisymmetric (−) combinations of the fields ϕ_α and θ_α:

$$H = H_+ + H_- + H_{+-}. \tag{6}$$

The three terms are given explicitly by:

$$\begin{aligned} H_+ &= \frac{u_+}{2\pi}\int dx \left[K_+ (\partial_x\theta_+)^2 + \frac{1}{K_+}(\partial_x\phi_+)^2\right] \\ &\quad + \int dx \frac{g_1}{(\pi a)^2}\cos(2\phi_+) \end{aligned} \tag{7}$$

$$\begin{aligned} H_- &= \frac{u_-}{2\pi}\int dx \left[K_- (\partial_x\theta_-)^2 + \frac{1}{K_-}(\partial_x\phi_-)^2\right] \\ &\quad + \int dx \left[\frac{g_2}{(\pi a)^2}\cos(2\phi_-) + \frac{g_3}{(\pi a)^2}\cos(2\theta_-)\right] \end{aligned} \tag{8}$$

and

$$H_{+-} = \int dx \frac{g_4}{(\pi a)^2}\cos(2\phi_+)\cos(2\phi_-), \tag{9}$$

where $\phi_\pm = \phi_1 \pm \phi_2$ and $\theta_\pm = (\theta_1 \pm \theta_2)/2$. (Note that the fields ϕ_+ and ϕ_- correspond to $\sqrt{2}\psi_1$ and $\sqrt{2}\psi_2$ in Ref. [12], respectively.) The naive continuum limit gives the following estimates for bare values of the coupling constants:

$$\begin{aligned} u_+ &= ta\sqrt{1 + \frac{U+6V}{\pi t}}, \quad K_+ = \frac{2}{\sqrt{1+\frac{U+6V}{\pi t}}} \\ u_- &= ta\sqrt{1 - \frac{U-2V}{\pi t}}, \quad K_- = \frac{2}{\sqrt{1-\frac{U-2V}{\pi t}}} \\ g_1 &= -g_2 = \frac{(2V-U)\,a}{2}, \; g_3 = -t\pi a, \; g_4 = Va \end{aligned} \tag{10}$$

To study the physical correlation functions we need to express the second quantized Bose operators on the lattice and the local site occupation in terms of the continuum fields. These relations are of the form

$$\begin{aligned} \frac{b(x)}{\sqrt{a}} &= \frac{A}{\sqrt{2\pi a}} e^{i\theta_+}\left[\cos(\theta_-) + ...\right] \\ \frac{n(x)}{a} &= \frac{1}{\pi}\partial_x\phi_+ + B\frac{(-1)^{\frac{x}{a}}}{\pi a}\sin(\phi_+)\cos(\phi_-) + ..., \end{aligned} \tag{11}$$

where A and B are non-universal constants and only the most relevant terms are shown. In general, the expansion of these operators also contains less relevant (subleading) terms.

The Hamiltonian H_+ of the symmetric degrees of freedom is similar to the usual low energy description of lattice bosons. The Umklapp term parameterized by g_1 is relevant for $K_+ < 2$. Here we consider the insulating phases, for which K_+ is indeed below this critical value[36]. The main difference from the standard bosonization of lattice bosons is that the parameter g_1 changes sign at $2V = U$. This change of sign marks a quantum phase transition from the MI, for which ϕ_+ is localized around zero, to another gapped phase in which it is localized near $\pm\frac{\pi}{2}$. As we shall see below, the latter turns out to be the HI phase and is characterized by string order. On the critical line, the system is described by a Luttinger liquid with power law correlations that depend on the non-universal parameter $\frac{1}{2} < K_+ < 2$. If K_+ is driven below $\frac{1}{2}$, the critical line becomes unstable, since the subleading term $\cos(4\phi_+)$ (which was omitted in Eq. (7)) becomes relevant. This possibility will be discussed further in Sec. II C. Note that the odd sector described by H_- is not critical. The term g_3 in (8) is relevant on both sides of the transition, so that the field θ_- is localized and remains massive at the critical point.

On the other hand, the transition from the HI to the DW phase is controlled by the odd sector. It occurs when the term $\cos(2\phi_-)$ becomes more relevant than the dual term $\cos(2\theta_-)$, that is when $K_- < 1$. According to the naive continuum limit the critical line is given by $V - 2U = 3\pi t$. This transition is of the Ising universality class[12,24]. This can also bee seen by refermionization of the Hamiltonian H_- at the critical point $K_- = 1$ and $g_2 = g_3$, which yields precisely the massless Majorana

fermions of the $1+1$ dimensional Ising model at criticality.

We remark that the precise values of the coupling constants as a function of the microscopic parameters are not simple to derive. The field theory (6) should be used to obtain the universal behavior of the system near the critical points which describe the quantum phase transitions, not to find the precise location of phase boundaries.

B. The string and parity order parameters

What is the physical distinction between the different insulating phases? It was shown in Ref. [6] that the HI phase of bosons is characterized by a non decaying string correlation function

$$\mathcal{O}_S^2 \equiv \lim_{|i-j|\to\infty} \left\langle \delta n_i \exp\left(i\pi \sum_{i\le k<j} \delta n_k \right) \delta n_j \right\rangle . \quad (12)$$

Here $\delta n_i \equiv n_i - \bar{n}$ is the deviation from the average (integer) filling $\bar{n}$. In section III we show that the MI phase is characterized by a different non local correlation function, which will be termed the "parity" correlation function

$$\mathcal{O}_P^2 \equiv \lim_{|i-j|\to\infty} \left\langle \exp\left(i\pi \sum_{i\le k<j} \delta n_k \right) \right\rangle . \quad (13)$$

For the sake of convenience, we define the parity and string operators

$$\hat{\mathcal{O}}_P(j) = \exp\left(i\pi \sum_{k<j} \delta n_k \right) \quad (14)$$

$$\hat{\mathcal{O}}_S(j) = \hat{\mathcal{O}}_P(j)\, \delta n_j, \quad (15)$$

such that $\mathcal{O}_P^2 = \lim_{|i-j|\to\infty} \left\langle \hat{\mathcal{O}}_P(i)\, \hat{\mathcal{O}}_P(j) \right\rangle$ and $\mathcal{O}_S^2 = \lim_{|i-j|\to\infty} \left\langle \hat{\mathcal{O}}_S(i)\, \hat{\mathcal{O}}_S(j) \right\rangle$.

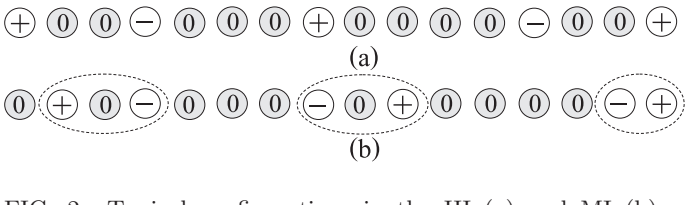

FIG. 2: Typical configurations in the HI (a) and MI (b) ground states. The numbers represent δn (the deviation of the local occupation from the average density). The HI can be described as a charge ordered $+,-,+,...$ state with an undetermined number of 0 sites between each $+$ and $-$. The MI is a dilute gas of particle-hole pairs (indicated by the dotted line).

A simple interpretation of these correlations is illustrated in Fig. 2. In both phases the ground state consists of configurations with most sites having precisely the average occupation, but also some particle and hole fluctuations. The parity $\mathcal{O}_P$ order in the MI phase implies that the fluctuations in this ground state are bound particle-hole pairs. On the other hand, the string order in the HI phase implies that a "renormalized" chain with all non fluctuating $\delta n_i = 0$ sites taken away would have density wave order (particle and hole fluctuations alternating along the chain). Physically, this can be understood as a compromises between the kinetic energy term in Eq. (1), which prefers maximum delocalization of particles and holes, and the nearest neighbor interaction term, which is minimized when particles and holes are neighbors. Indeed, the HI phase is realized at intermediate values of V/t.

Within the effective field theory the HI and MI seem to differ only in the expectation value of the field ϕ_+ which is pinned in each of these phases. It is interesting to relate this distinction to the string and parity correlations that characterize the two phases. Since both order parameters contain the factor $\exp\left(i\pi \sum_{i<k<j} \delta n_k\right)$, we may naively expect their bosonized forms to contain $\exp\left[i\phi_+(x)\right]$, since $\sum_{i<k<j} \delta n_k \to \frac{1}{\pi}\int_{x_i}^{x_j} dx \partial_x \phi_+ = \frac{1}{\pi}\left[\phi_+(x_j) - \phi_+(x_i)\right]$. However, the exponential should be symmetrized carefully to obtain a hermitian operator. In Appendix C, we argue for the following forms of $\hat{\mathcal{O}}_S$ and $\hat{\mathcal{O}}_P$ in the bosonized theory:

$$\hat{\mathcal{O}}_S(x) \sim \sin\left(\phi_+(x)\right) \quad (16)$$

$$\hat{\mathcal{O}}_P(x) \sim \cos\left(\phi_+(x)\right) \quad (17)$$

Here the form of (16) was postulated on the basis of symmetry. For a more microscopic derivation see Refs. [26,29].

The above expressions for the string and parity correlations are consistent with the respective phases derived from Eq. (7,8). The MI phase corresponds to $g_1 < 0$, which implies a non vanishing expectation value of the parity operator $\langle \cos(\phi_+(x)) \rangle \neq 0$. The fact that ϕ_+ is locked to 0 or π in this phase is consistent with the particle density being concentrated on the lattice sites, as in the cartoon product state $|\Psi_{MI}\rangle \sim \prod_j b_j^\dagger |0\rangle$. In the HI phase on the other hand $g_1 > 0$, so that $\langle \sin(\phi_+(x)) \rangle \neq 0$ and therefore non vanishing string order. Here ϕ_+ is locked to $\pi/2$ or $3\pi/2$, which implies a shift of the particles by half a lattice constant compared with the MI, that is, the density is centered on the links rather than the lattice sites. This is captured by the cartoon wave function $|\Psi_{HI}\rangle \sim \prod_j (b_j^\dagger + b_{j+1}^\dagger)|0\rangle$, which is closely analogous to the AKLT state that describes a valence bond solid in spin-1 chains.

C. Coupling to symmetry breaking perturbations

A realization of the phases described above with ultracold atoms would open up new ways to probe the nature of string and parity orders by how they react to different perturbations. Interestingly, we shall see that in spite of being highly non local, the string and parity operators nevertheless couple in interesting ways to local symmetry breaking fields.

As compared to the spin chain model [Eq. (4)], an inherent broken symmetry in the microscopic Hamiltonian (1) is the absence of particle hole symmetry $\delta n_i \to -\delta n_i$. The spin model does enjoy the analogous symmetry associated with rotation by π around the y axis, which takes $S^z \to -S^z$ and $S^x \to -S^x$. Nevertheless both systems are described by the same low energy field theory (6). Terms that break just the particle hole symmetry, such as $\partial_x\phi(\partial_x\theta)^2$, are irrelevant at the HI-MI critical point, and do not change either the parity $\langle \cos(\phi_+)\rangle$ or string $\langle \sin(\phi_+)\rangle$ order parameters in the insulating phases. What are the minimal perturbations that eliminate the sharp distinction between these two phases and gap out the critical point separating them?

Consider the following perturbation of the Hamiltonian (7):

$$\begin{aligned} H_+ + \lambda\hat{P} &= H_+ + \lambda \int \frac{dx}{(\pi a)^2}\sin(2\phi_+) \\ &= H_{LL} + \tilde{g}\int \frac{dx}{(\pi a)^2}\cos(2\phi_+ + \chi). \quad (18) \end{aligned}$$

Here H_{LL} is the critical Luttinger liquid theory at the transition and $\chi = \arctan(\lambda/g_1)$ and $\tilde{g} = \sqrt{g_1^2+\lambda^2}$. Clearly $\hat{P}$ is a relevant perturbation at the critical point, leading to a gapped state even when the parameter g_1 crosses zero, where the critical point would have been.

Note that the operator $\hat{P}$ breaks both the particle hole and lattice inversion symmetries. This is seen for example in the representation of the single chain as two coupled fermionic chains (as in Ref. [12]). Written in terms of the fermions the perturbation is

$$\sin(2\phi_+) \sim i\psi^\dagger_{R,1}\psi^\dagger_{R,2}\psi_{L,1}\psi_{L,2} + H.c., \qquad (19)$$

where $\psi_{R,\alpha}$ and $\psi_{L,\alpha}$ for $\alpha = 1,2$ are the right and left moving fermions in the two fermionic chains, respectively. (Note that the two chains labelled by α are the two fictitious spin-1/2 chains discussed in the paragraph preceding Eq. (5).) This term is clearly odd under inversion (which changes $\psi_{R,\alpha} \longleftrightarrow \psi_{L,\alpha}$) and particle-hole ($\psi^\dagger_{R/L,\alpha} \longleftrightarrow \psi_{R/L,\alpha}$) transformations, and even under time-reversal.

The perturbation $\hat{P}$ can be viewed as a local polarizing field that induces a small "dipole" moment on every lattice site. (By "dipole" we mean $\int xn(x)dx$, i.e. the electric dipole moment that we would get if the particles where charged. It is not related to the real moment of the dipolar atoms.) It is clear from the second line of (18) that the term $-\tilde{g}\cos(2\phi_+ + \chi)$ acts to lock the field ϕ_+ to the values $\phi_+ \approx -\chi/2$ or $\phi_+ \approx \pi - \chi/2$. The density concentration is shifted accordingly by $\sim (\chi/2\pi)a$ away from the lattice points, resulting in a local dipole moment at these points. The shift of $-\chi/2$ also implies that both parity $\langle\hat{\mathcal{O}}_P\rangle$ and string $\langle\hat{\mathcal{O}}_S\rangle$ order parameters gain a finite expectation value in the presence of this perturbation. Hence the sharp distinction between the Mott and Haldane insulating phases is lost. It is interesting to note in this regard the similar effect of a symmetry breaking field on a conventional quantum phase transitions involving spontaneous breaking of that symmetry. The field gaps out the critical point while inducing a non vanishing order parameter in the disordered phase. It is remarkable that breaking inversion symmetry has this effect in the HI-MI transition despite the fact that neither phase has broken lattice inversion symmetry (at least in an infinite system or in a finite system with periodic boundary conditions).[35]

We note that the converse is also true: a finite expectation value of both parity and string orders immediately entails broken inversion symmetry in the ground state. This is seen by writing the local symmetry breaking field as a product of the two non local order parameters $\sin(2\phi_+) = 2\sin(\phi_+)\cos(\phi_+)$.

The connection between the string and parity correlations and the breaking of inversion symmetry can also be understood from the microscopic viewpoint sketched in Fig. 2. A non-zero expectation value of the parity operator $\langle\hat{\mathcal{O}}_P\rangle$ is associated with pairing of particle and hole fluctuations in the ground state, while $\langle\hat{\mathcal{O}}_S\rangle \neq 0$ corresponds to alternate ordering of the particle and hole fluctuations. Having both implies organization of the particle hole pairs in the form of ordered dipoles. A cartoon wave-function capturing this mixed phase is given by:

$$|\,\Psi_d\,\rangle = \prod_i \left[(1+d)b_i^\dagger + (1-d)b_{i+1}^\dagger\right]|\,0\,\rangle \qquad (20)$$

Changing d between 0 and 1 facilitates a continuous connection between the MI and HI phases.

In an optical lattice system it is relatively easy to apply a perturbation that breaks lattice inversion symmetry. A second laser with double the wavelength can be used to produce a lattice of asymmetric double wells[33,34]. Terms such as $\sin(2\phi_+)$ are then allowed by symmetry and will therefore be imminently generated in the effective field theory.

An intriguing question that naturally arises is whether a phase described by a wave-function such as Eq. (20) can occur by spontaneous breaking of inversion symmetry. In fact, there is a natural route by which such symmetry breaking can take place. As discussed in Sec. II A, the critical line between the MI and HI phases is stable when $K_+ > \frac{1}{2}$. For $K_+ < \frac{1}{2}$ sub-leading terms, such as $\cos(4\phi_+)$, become relevant and open a gap that would stabilize a new phase. In particular, if the coefficient of the $\cos(4\phi_+)$ term is positive, the ϕ_+ field is locked

to $\pm\pi/4$, which implies spontaneously broken inversion symmetry. In this case, the particles (or density maxima) are effectively pinned to a point which is either 1/4 lattice spacing to the left or to the right of lattice sites. What microscopic interactions are required to stabilize such a phase is an open question. It can only occur if the value of the Luttinger parameter K_+ goes below $\frac{1}{2}$ before the transition to the DW terminates the critical line separating the MI and HI phases. This point will be investigated in a later study.

A completely different type of perturbation that is difficult to realize in cold atom systems, but is nevertheless worth mentioning, is one that breaks the $U(1)$ symmetry associated with number conservation. Such a perturbation can be added to the continuum theory (7) as a term of the form $\lambda \int dx \cos(\theta_+)$. In the spin chain case [Eq. (4)], this term corresponds to a transverse magnetic field. Clearly, this perturbation is relevant and would gap out the critical point. Inside the HI and MI this term produces a finite density of kinks in the field ϕ_+ and therefore leads to vanishing of both expectation values $\langle\cos(\phi_+)\rangle$ and $\langle\sin(\phi_+)\rangle$. Again the sharp distinction between the HI and MI phases is lost.

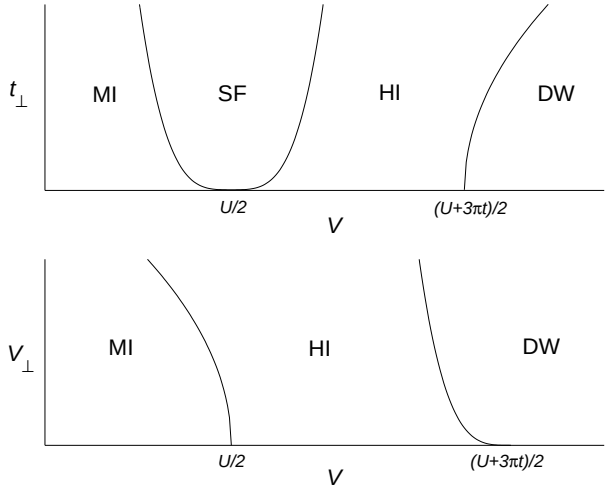

FIG. 3: Evolution of the phase diagram with inter-chain coupling predicted from bosonization. (a) Plane of the nearest neighbor interaction V versus $t_\perp$ (inter-chain tunneling) at fixed on-site interaction U and no inter-chain repulsion. (b) In the plane of V versus $V_\perp$ (inter-chain repulsion) at $t_\perp = 0$ and fixed U.

D. Continuum limit of weakly coupled chains

We move on to discuss a system of two coupled EBHM chains described by the microscopic Hamiltonian (3). The starting point for a low energy description at weak inter-chain coupling are the decoupled single chain field theories (6) which involve four bosonic fields, $\phi_{\alpha,\pm}$ (with $\alpha = 1, 2$ a chain index) and their canonical conjugate fields $\theta_{\alpha,\pm}$.

The continuum limit of the inter-chain Hamiltonian (2) is now conveniently written in terms of symmetric and anti-symmetric combinations of the *even* fields of each chain: $\Phi_\pm = (\phi_{1,+} \pm \phi_{2,+})/\sqrt{2}$, and $\Theta_\pm = (\theta_{1,+} \pm \theta_{2,+})/\sqrt{2}$:

$$\begin{aligned} H_{V_\perp} &= \int dx \{ \frac{g_5}{2\pi^2} \left[(\partial_x \Phi_+)^2 - (\partial_x \Phi_-)^2 \right] \\ &+ \frac{g_6}{(\pi a)^2} \left(\cos\left(\sqrt{2}\Phi_-\right) - \cos\left(\sqrt{2}\Phi_+\right) \right) \\ &\times \cos(\phi_{1,-}) \cos(\phi_{2,-}) + ... \} \end{aligned} \tag{21}$$

$$\begin{aligned} H_{t_\perp} &= \int dx \frac{g_7}{(\pi a)^2} \cos\left(\sqrt{2}\Theta_-\right) \\ &\times \left[\cos(\theta_{1,-}) \cos(\theta_{2,-}) + ... \right] \end{aligned} \tag{22}$$

where the bare values of the parameters are $g_5 = V_\perp a$, $g_6 = V_\perp a B^2$ and $g_7 = -t_\perp \pi a A^2$. (Here A, B are the non-universal constants that appear in Eq. (11).) We shall analyze how these terms affect the low energy physics of the decoupled chains (6) in the limit of weak $t_\perp$ and $V_\perp$.

The HI phase – The simplest case to consider is the case where the decoupled chains are in the HI phase. Because of the finite gap in each chain's spectrum, any inter-chain coupling term is irrelevant in this case, which implies that the chains remain essentially decoupled at weak coupling. Nevertheless, since the string order parameter is a non local object in terms of either the density or the phase field it is destroyed by infinitesimal inter-chain tunneling. In appendix A we show that the string correlations decay exponentially with a correlation length that scales as $(\Delta/t_\perp)^2$, where Δ is the gap (see also Ref. [18]). It is easy to understand this effect by considering the low energy theory (6) with the perturbation (22). In the HI phase of a single chain the the field ϕ_+ is localized near $\pm\pi/2$, so that the string order parameter $\langle\sin(\phi_+)\rangle$ is fixed around ± 1. However, the perturbation $t_\perp \cos\left(\sqrt{2}\Theta_-\right)$, which hops a particle from one chain to the other, induces a kink in the string order parameter of each chain. Therefore at any finite coupling strength this perturbation destroys the string order by creating a finite density $\propto (t_\perp/\Delta)^2$ of kinks in the Z_2 order parameter.

We note that the product of the string operators on the two chains remains invariant to the inter-chain tunneling because this perturbation always creates a kink on one chain and an anti-kink on the other. It is therefore tempting to define the product $O_{SL} = \sin(\phi_{+,1}) \sin(\phi_{+,2})$ as a generalized string order parameter for the ladder. Such an operator still has a non-zero expectation value in the HI phase when inter-chain hopping is introduced. However, it gains a finite expectation value also in the MI phase in the presence of a finite $t_\perp$ and therefore cannot serve to distinguish these two phases. To see this we consider the decoupled chains in the MI phase $\phi_{+,\alpha} \approx 0$. The action of the inter-chain tunneling operator at point x produces a kink-anti kink pair corresponding to a change of $\phi_{+,1}$ from 0 to π at x and of $\phi_{+,2}$ from 0 to $-\pi$. At

the point x the values of the fields are $\phi_{+,1} \approx \pi/2$ and $\phi_{+,1} \approx -\pi/2$, therefore such a point contributes -1 to the product string operator. We therefore expect that in the presence of finite coupling $t_\perp$ the product string operator would gain an expectation value even in the MI phase, which is of the order of the kink density $(t_\perp/\Delta)^2$.

It is natural to ask what is the fate of the quantum phase transition from the MI to HI phase in the two chain system where we cannot define a clear cut distinction between the two phase.

HI to MI transition – The critical theory for this transition is a Luttinger liquid described by H_+, Eq. (7), with $g_1 = 0$. In this region, H_- is gapped, with the $\cos(2\theta_{\alpha,-})$ term more relevant than the $\cos(2\phi_{\alpha,-})$ term. We may therefore assume that the $\theta_{\alpha,-}$ fields are pinned at the minimum of the cosine potential. The effective low energy Hamiltonian in the $\Phi_\pm$ sector is written as follows:

$$\begin{aligned} H_{MI\to HI} &= \sum_\pm \int dx \frac{\tilde{u}_\pm}{2}\left[\tilde{K}_\pm (\partial_x \Theta_\pm)^2 + \frac{1}{\tilde{K}_\pm}(\partial_x \Phi_\pm)^2\right] \\ &+ \int dx \frac{g_1}{(\pi a)^2}\cos\left(\sqrt{2}\Phi_+\right)\cos\left(\sqrt{2}\Phi_-\right) \\ &+ g_7 \int dx \frac{1}{(\pi a)^2}\cos\left(\sqrt{2}\Theta_-\right), \end{aligned} \tag{23}$$

where the bare values are $\tilde{u}_\pm = u_\pm\sqrt{1 \pm \frac{2g_5 K_+}{\pi u_+}}$, $\tilde{K}_\pm = K_+/\sqrt{1 \pm \frac{2g_5 K_+}{\pi u_+}}$, and $g_7 \propto t_\perp$. Here we have replaced $\cos(\theta_{\alpha,-})$ by its non-zero expectation value. Note also that since the fields $\theta_{\alpha,-}$ are pinned, the $g^{(2)}_{v_\perp}$ term in Eq. (21) (which contains $\cos(\phi_{\alpha,-})$) is strongly irrelevant at this critical point, and therefore it was omitted in Eq. (23). We will, however, consider its effect on the phase diagram in what follows.

The Hamiltonian (23) is identical to the effective Hamiltonian derived in Ref. [14] for a system of two Bose-Hubbard chains coupled by an inter-chain hopping term. The only difference is that here, due to the extended interaction terms, a wider regime of parameters is accessible in Eq. (23). Of particular interest is the transition point from the HI to the MI phase, where $g_1 = 0$ (which was only possible in the non-interacting limit in Ref. [14]).

For completeness, we will now review briefly the RG analysis of $H_{MI\to HI}$ in Eq. (23), following Ref [14]. The leading order RG flow equations are:

$$\begin{aligned} \frac{dg_1}{d\ell} &= \left(2 - \frac{\tilde{K}_+}{2} - \frac{\tilde{K}_-}{2}\right) g_1 \\ \frac{dg_7}{d\ell} &= \left(2 - \frac{1}{2\tilde{K}_-}\right) g_7 \\ \frac{d\tilde{K}_+}{d\ell} &= -\frac{K_+^2 g_1^2}{16\pi^2} \\ \frac{d\tilde{K}_-}{d\ell} &= -\frac{K_+^2 g_1^2}{16\pi^2} + \frac{g_7^2}{8\pi^2} \end{aligned} \tag{24}$$

The fate of the system is determined by the competition between the g_7 and g_1 terms, which contain the dual cosine terms $\cos\left(\sqrt{2}\Theta_-\right)$ and $\cos\left(\sqrt{2}\Phi_-\right)$, respectively. If g_1 dominates, then the system will be in a HI-like phase (for $g_1 > 0$) or an MI-like phase (for $g_1 < 0$). If g_7 dominates, then a new phase is stabilized. Note that at the $g_1 = 0$ critical point, the g_7 term is relevant for $\tilde{K}_- > \frac{1}{8}$.

We can use the flow equations (24) to determine the form of the phase boundaries that separate the new $\tilde{g}_{t_\perp}$ dominated phase from the HI and MI phases. Imagine that we start from a point on the critical line between the MI or HI and the large $\tilde{g}_{t_\perp}$ phases, $(\tilde{g}_{t_\perp,c}, g_{1,c})$, where both $\tilde{g}_{t_\perp,c}$ and $g_{1,c}$ are small. Integrating the leading order flow equations, we find that this point is mapped to the point $\left(t_{\perp,c}(\Lambda_0/\Lambda)^{2-1/\left(2\tilde{K}_-\right)}, g_{1,c}(\Lambda_0/\Lambda)^{2-\tilde{K}_+/2-\tilde{K}_-/2}\right)$, where $\Lambda_0/\Lambda > 1$ is the RG scaling factor. Clearly, this point must also be on the critical line. Therefore the critical line must be of the form[14] $t_{\perp,c} \propto |g_{1,c}|^\alpha$ where $\alpha = \frac{2-1/\left(2\tilde{K}_+\right)}{2-\tilde{K}_+/2-\tilde{K}_-/2}$. For weak to intermediate interactions, this gives $\alpha > 1$.

To elucidate the nature of the new phase that forms between the Mott and Haldane insulators for non-vanishing $t_\perp$, we consider the possible sub-leading interactions that may become relevant in this phase. The single chain even sector Hamiltonian H_+ (Eq. (7)) can contain higher harmonics of the form $\cos(2n\phi_{\alpha,+})$ with $n > 1$. However, when expanded in terms of $\Phi_\pm = (\phi_{1,+} \pm \phi_{2,+})/\sqrt{2}$, these terms are seen to be irrelevant since they always contain the odd field Φ_-, whose conjugate Θ_- is pinned. The term $\cos\left(\sqrt{8}\Phi_+\right)$ can also be generated to higher orders in the bare couplings. (For example, such a term is generated during the RG flow to second order in g_1.) This term has a scaling dimension of $2\tilde{K}_+$, therefore it is relevant for $\tilde{K}_+ < 1$. This represents a strong interaction, therefore one may still expect that for small to moderate U, V and inter-chain coupling, this term would be irrelevant. In that case, the intermediate finite $t_\perp$ phase is gapless, and characterized by power law correlations. Using the bosonized expression for the boson creation operator [Eq. (11)], the off-diagonal correlation function in this phase is

$$\langle b_\alpha(x)^\dagger b_\beta(0)\rangle \sim \langle e^{i\Theta_+(x)/\sqrt{2}} e^{-i\Theta_+(0)/\sqrt{2}}\rangle \sim \frac{1}{|x|^{\frac{1}{4\tilde{K}_+}}} \tag{25}$$

where we have replaced $\cos(\theta_{1,2-})$ and $\cos(\sqrt{2}\Theta_-)$ by their non-zero expectation values. Therefore, $\tilde{K}_+$ can be estimated numerically in the gapless phase by measuring the power law decay of this correlation function. We conclude that the phase penetrating between the HI and MI at finite $t_\perp$ is a SF phase which remains stable as long as the above correlation function decays with a power smaller than $\frac{1}{4}$.

In Ref. [14] it was found that turning on inter chain

tunneling between two chains that are in the MI phase can drive a transition to a superfluid at a critical value of $t_\perp$. Here we showed how this transition drops to $t_\perp = 0$ as one approaches the MI-HI critical point.

The actual value of the Luttinger parameter $\tilde{K}_+$ can be calculated reliably only in the weak coupling regime. To estimate it for strong coupling we use numerical DMRG simulations (Section III). If either the intra-chain U, V or the inter-chain $V_\perp$ are increased sufficiently, $\tilde{K}_+$ can be driven below the critical value of 1. Then the system would undergo a Kosterlitz-Thouless (KT)-type transition to an insulating phase.

We finally note that in the limit of vanishing inter-chain tunneling $t_\perp = 0$, but finite interaction $V_\perp \neq 0$, no intermediate SF phase is formed near the MI to HI phase boundary. The inter-chain coupling is in this case marginally irrelevant at the critical point, affecting only a renormalization of the Luttinger parameter.

HI to DW transition – This transition is of the Ising universality class[12,24]. It is controlled by the odd sector single chain Hamiltonian H_- [Eq. (8)], which describes a competition between the terms $\cos(2\theta_-)$ and $\cos(2\phi_-)$. The transition to the DW phase occurs when the latter term becomes more relevant, which for small g_2, g_3 happens at $K_- = 1$. For this value of K_- the theory (8) can be refermionized and written as a quadratic Hamiltonian of Dirac fermions with a mass term proportional to g_2 and a pairing term proportional to g_3. The model is diagonalized when formulated in terms of two Majorana fields[25]. At the critical point $g_2 = g_3$ (and $K_- = 1$), one of these Majorana fields becomes massless. A massless Majorana theory is equivalent to an Ising critical point.

$H_{t_\perp}$ is clearly irrelevant at the critical point, since it contains $\cos\left(\sqrt{2}\Theta_-\right)$ while the dual field Φ_- is pinned. The only effect this term could have is a slight bending of the HI to DW phase boundary.

On the other hand we show below that $H_{V_\perp}$ is a relevant perturbation at the Ising critical point. First we can replace the operator $\cos(\sqrt{2}\Phi_-) - \cos(\sqrt{2}\Phi_+)$ appearing in $H_{V_\perp}$ by its non-zero expectation value. (Note that these operators involve only the even modes $\phi_{\alpha,+}$ of each chain, and the even sector Hamiltonian is not close to its critical point.) Now in order to determine the scaling dimension of $H_{V_\perp}$, we need the scaling dimension of the operators $\cos\left(\phi_{1/2,-}\right)$ at the critical point. As mentioned above, there is a correspondence, via the mapping to a the Majorana theory, between these operators and the two Ising models that describe the odd sector Hamiltonain close to the critical point. The $\cos\left(\phi_{1/2,-}\right)$ operators correspond to products of the spin operators of the two Ising models[23,27]. However since only one of these Ising models becomes critical at the transition from HI to DW the operator $\cos\left(\phi_{1/2,-}\right)$ has the scaling dimension of Ising spins in $1+1$ dimensions at criticality, which is $1/8$. $H_{V_\perp}$ is thus strongly relevant. This can also be understood simply by the fact that at the transition to the DW phase, the density wave susceptibility of each chain diverges, and therefore the density-density coupling between the two chains is strongly relevant. $H_{V_\perp}$ then drives a transition to a density ordered phase with the order parameters of the two chains locked to each other. The high $V_\perp$ phase is thus not distinct from the $V_\perp = 0$ DW phase.

The HI-DW phase boundary at finite $V_\perp$ can be obtained using the same scaling argument as we used before for the phase boundary between the HI or MI and the large $t_\perp$ phases. This gives that near the $V_\perp = 0$ critical point, the critical line is of the form $V_{\perp,c} \propto (V_c - V)^{7/4}$, where V_c is the critical value for the transition of the single chain from the HI to the DW phase (which is $V_c = (U + 3\pi t)/2$ in the weak coupling limit).

In this section we studied weak coupling between two chains. The main results are summarized in the phase diagram plotted in Fig. 3. The case of an infinite array of chains is not expected to yield qualitatively different results in the weak inter-chain coupling limit. The main difference would be that the intermediate superfluid state would in this case support true long range order instead of power-law correlations.

III. DMRG RESULTS

In this section we present numerical results to support the predictions of the field theoretical analysis from the previous sections. To this end we compute the ground state and lowest excitations of the extended Bose Hubbard model (1) and (2), using the Density Matrix Renormalization Group (DMRG)[31]. The section is organized as follows. We first treat the case of a single unperturbed chain (Sec. III A) at filling of $\bar{n} = 1$ boson per site. Expanding on the results of Ref. [6], we focus on the interplay of the non local string and parity correlations near the transition between the MI and HI phases. In Sec. III B we investigate how a perturbation that breaks the lattice inversion symmetry affects the MI-HI phase transition. We find that such a perturbation gaps out the critical point and thus eliminates the phase transition, in agreement with the field theoretical prediction. In Sec. III C we move on to address a two-leg ladder with only interaction coupling between the two chains. Finally in Sec. III D we analyze the two leg ladder with tunnel coupling. As expected we find that this coupling leads to an intermediate superfluid phase between the Mott and Haldane insulators.

Before proceeding let us give the essential technical details of the numerical calculations. To expand the domain of the HI phase we add to (1) the next-nearest neighbor interaction $(V/8)\sum_i \delta n_i \delta n_{i+2}$. The DMRG calculations are performed with open boundary conditions, while keeping $m = 250$ states per block. As usual in bosonic problems, we also need to truncate the Fock space of site occupations. For calculations presented in this section we allow the four occupation states $n = 0, 1, 2, 3$. Including one more occupation state per site had a negligible effect on the results in a sample of representative calcula-

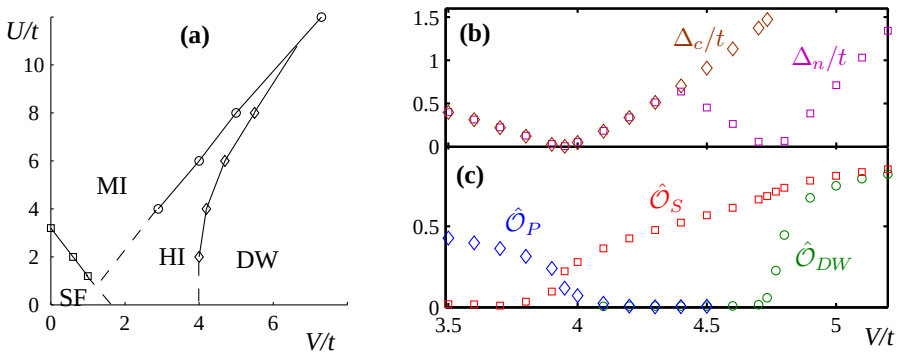

FIG. 4: (Color online.) (a) Phase diagram of a single unperturbed chain in the space of $(U/t, V/t)$, obtained from the numerical calculations. (b) The "charge" ($\diamond$) and "neutral" ($\square$) gaps along the same cut through the three insulating phases. The charge gap vanishes at the MI-HI transition, whereas only the "neutral" gap vanishes at the transition to the DW phase. (c) The parity ($\diamond$), string ($\square$) and Density wave (o) order parameters as a function of V/t along a line of constant $U/t = 6$. The string and parity orders are defined as the square roots of (12) and (13) respectively.

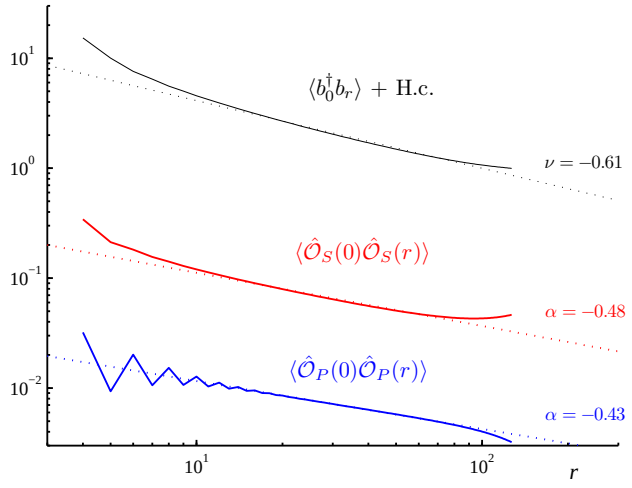

FIG. 5: (Color online.) Decay of the parity and string correlations, and of the single particle density matrix at the HI-MI transition. The power-law fits are consistent with the field theoretical predictions for the relations between the different decay exponents (see text).

tions. The maximum number of sites in the calculations was 256, including chains of length $L = 256$ and two leg ladders of $L = 128$.

A. Unperturbed single chain

To map the phase diagram of a single chain (Fig. 4(a)) we compute the parity, string, and Density wave (DW) correlations in the ground state. The long distance behavior of these correlations as a function of V for a particular value of the on-site interaction U is plotted in Fig. 4(c). As expected, the MI is characterized by non vanishing Parity "order", the HI by string order, and the DW phase by non decaying density correlations. The finite value of the string and parity correlations seen in the figure at the MI-HI critical point is due to the finite system size ($L = 256$). The field theoretical analysis predicts power-law decay of these correlation functions with a non universal power α, which is directly related to the decay exponent ν of the single particle density matrix via the relation $\alpha = 1/(4\nu)$. Along the line of critical points separating the HI and MI phases the exponents are predicted to run in the range $1/4 < \nu < 1$. These predictions are consistent with the power-law fits of the relevant correlation functions at the critical point, as presented in Fig. 5 (See explanation below on how the critical point is located in the calculations).

Also shown in Fig. 4(a) is the superfluid (SF) phase at low U, V, which is identified by measuring the decay exponent of the single particle density matrix ν. The SF phase is stable when $\nu < 1/4$.

In addition to ground state correlations we compute the gap to "charged" and "neutral" excitations. The neutral excitation gap Δ_n is obtained by targeting the lowest excitation in the sector with exactly $\bar{n} = 1$ particles per site. The "charge" gap is defined by $\Delta_c = E_0(+1) + E_0(-1) - 2E_0(0)$, where $E_0(\pm 1)$ are the ground state energies of the system with one more/less particle. There is an interesting complication in extracting the bulk gap in the HI phase. For open boundary conditions this phase supports low energy edge excitations. We can identify these states by inspecting the density profile of the wave functions. The appearance of the edge states coincides with the transition to the HI phase and facilitates the most precise determination of the transition point in a finite system. In most cases, however, we are interested in the bulk properties. To extract the bulk "charge" and "neutral" gaps, we lift the edge excitations to high energy by applying a sufficiently strong field at the edges: $V_{edge}(\delta n_1 - \delta n_L)$. The gaps are plotted in Fig. 4(b) for a cut of the phase diagram at constant $U/t = 6$. It is seen that both the "charge" and "neutral" gaps van-

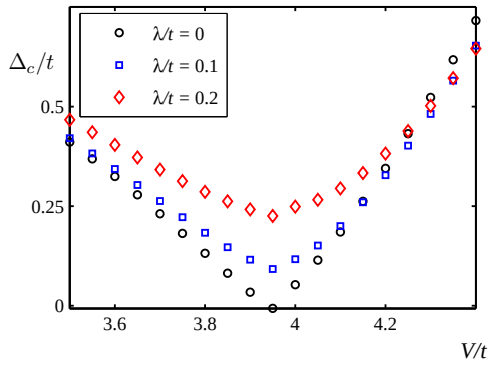

FIG. 6: (Color online.) Charge gap as a function of V/t at constant $U/t = 6$ for different values of the inversion-symmetry breaking perturbation. λ is defined in (26).

ish at the transition from the MI to the HI phase. On the other hand only the "neutral" gap vanishes at the transition from the HI to the DW phase.

B. Breaking of lattice inversion symmetry

Following the predictions of section II C we add the term

$$\delta H = \lambda \sum_i (\delta n_i b_i^\dagger b_{i+1} + H.c.) \qquad (26)$$

to the Hamiltonian (1). This is one of the simplest terms that break the lattice inversion symmetry. Based on the predictions of II C we expect that the quantum critical point separating the HI and MI phases would be eliminated in the presence of this term and an adiabatic connection between the HI and MI would be facilitated. This is indeed what is seen from the calculated charge gap in the presence of the perturbation. In Fig. 6 we plot the charge gap along a cut through the phase diagram with $U/t = 6$, as a function of V/t. We see that for a non vanishing value of λ the gap does not vanish and the phase transition is eliminated.

C. Two leg ladder with inter-chain repulsive interaction

We move on to treat two leg ladders. The simplest coupling between two chains is via the density-density interaction $V_\perp \sum_i n_{1,i} n_{2,i}$. The field theoretical analysis predicted that this interaction is marginal at the transition between the MI and HI phases. In other words it leaves the transition in tact, affecting only a renormalization of the Luttinger parameter which controls the decay of the single particle density matrix at the critical point.

At the transition from HI to DW the interaction coupling $V_\perp$ is expected to shift the critical point to lower

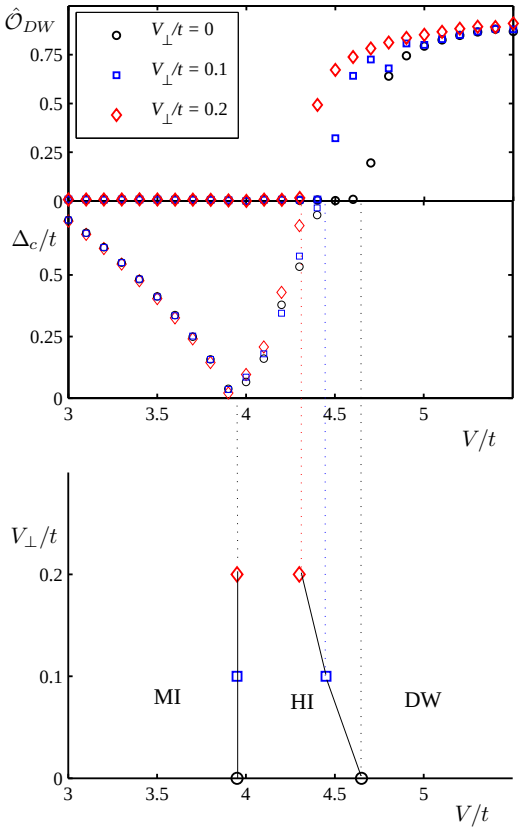

FIG. 7: (Color online.) *Effect of inter-chain interaction coupling on the phase diagram.* (a) Calculated DW order parameter as a function of V/t at constant $U/t = 6$ for different values of the interchain interaction $V_\perp$. (b) Calculated charge gap on the same cut through the phase diagram and the same values of $V_\perp$. (c) Evolution of the phase boundaries with $V_\perp$ inferred from the calculations.

values of V. The change in both phase boundaries with increasing $V_\perp$ are plotted in Fig. 7. The transition points are inferred from the vanishing of the "charge" gap at the MI-HI transition and the emergence of DW order.

D. Two leg ladder with Inter-chain tunnel coupling

Finally we include the inter-chain tunneling $-t_\perp \left(b_{A,i}^\dagger b_{B,i} + \text{H.c.}\right)$. According to the field theoretical analysis of the previous sections this is a relevant coupling at the MI-HI critical point. An intermediate phase is predicted to occur between these two insulators. In fact the intermediate phase is expected to be a superfluid if the parameter $K_+ > 1$. It would seem that rather strong interactions are required to violate this criterion. However we note that K_+ may be highly renormalized and not easily estimated from the

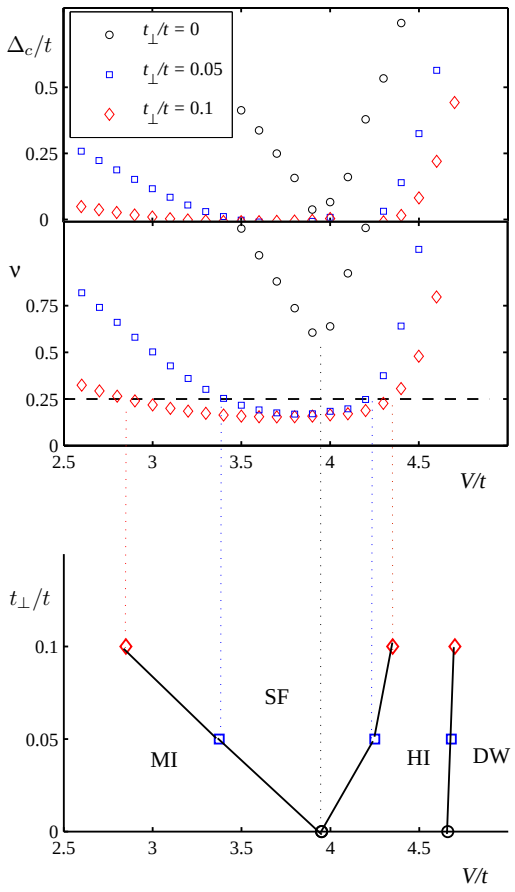

FIG. 8: (Color online.) *Effect of inter-chain tunnel coupling on the phase diagram.* (a) Calculated charge gap as a function of V/t at constant $U/t = 6$ for different values of the inter-chain tunneling $t_\perp$. The gaps were obtained by extrapolation to an infinite chain through finite size scaling analysis. The fact that the estimate for the gap are sometimes slightly negative is due to errors in the extrapolation. Note the gapless phase that appears between the two insulating phases. (b) Power-law fit for the spatial decay of the single particle density matrix for the same cuts through the phase diagram. The fact that $\nu < 1/4$ in the gapless phase confirms that it is indeed a superfluid. The transition to the gapped phase seems to occur at the universal exponent $\nu = 1/4$ consistent with a Kosterlitz-Thouless transition. (c) Evolution of the phase boundaries with $t_\perp$ inferred from the calculations.

microscopic parameters. Therefore only the numerical calculations presented in this section can confirm the nature of the intermediate phase.

The results of the calculations are summarized in Fig. 8. The charge gap is shown as a function of V/t in a cut through the phase diagram at constant U/t. For increasing $t_\perp$ we see a that a gapless phase opens up between the MI and HI phases. Up to numerical accuracy and finite size effects the results are consistent with the prediction that the gapless phase is established for any non vanishing value of $t_\perp$. The exponent ν with which we fit the decay of the single particle correlation function is shown as a function of V/t. The fact that $\nu < 1/4$ in the domain of vanishing gap is consistent with a superfluid phase which is destabilized in a KT transition on crossing to either the HI or MI phases. We note that we find similar result also for different values of U/t for which the HI phase can be realized.

IV. SUMMARY AND DISCUSSION

The purpose of this work was to investigate fundamental problems concerning the nature of non local string order parameters, which were brought into focus by the possible realization in systems of ultracold atoms[6]. In particular we addressed the question of how static perturbations, which couple to *local* physical operators can nonetheless influence quantum phases and phase transitions that involve the highly *non-local* order parameter.

A key result of this analysis is the discovery of a surprising connection between the string order and breaking of the lattice inversion symmetry (Note that breaking of particle-hole symmetry is also needed – but this is anyway broken at the outset in the Bose system). In the context of this work the two phases that are characterized by a non local order parameter are the Haldane insulator, which sustains string order, and the Mott insulator, which supports non zero expectation of the parity operator. We find that a perturbation which breaks the lattice inversion symmetry gaps out the critical point between the two phases. Correspondingly the sharp distinction between them is eliminated, in the sense that non vanishing string order is induced in the Mott phase and parity expectation value in the Haldane phase. This is similar to the effect of a symmetry breaking perturbation on a conventional phase transition involving spontaneous breaking of *the same* symmetry. But curiously, neither the Mott or Haldane phase involve spontaneous breaking of the lattice inversion symmetry.

The seemingly mysterious connection between lattice inversion symmetry and the string operators is elucidated by the effective long wavelength description of the problem. The symmetry breaking field $\sin(2\phi_+)$ has the symmetries of a local dipole field: it is odd under both lattice inversion and particle-hole transformations. Incidentally, this operator can also be decomposed as a product of the long wavelength expressions for the string $\sin(\phi_+)$ and parity $\cos(\phi_+)$ operators. Thus in each phase only one (non local) factor of the local "dipole" field gains an expectation value and so inversion symmetry remains intact. But this also implies that in each of these phases the external perturbation becomes in effect a direct coupling to the non local order parameter of the other phase. For example in the MI phase where $\langle\hat{\mathcal{O}}_P\rangle = \langle\cos\phi_+\rangle > 0$ we have that $\lambda \sin 2\phi_+ \approx \lambda\langle\hat{\mathcal{O}}_P\rangle\hat{\mathcal{O}}_S$, which is essentially an ordering field for the string order.

It is relatively easy to apply such a symmetry breaking field in an optical lattice realization of the transi-

tion from Mott to Haldane insulator. The principle has already been demonstrated successfully in experiments that created a lattice of asymmetric double wells using a secondary laser with half the wavelength of the main laser[33,34]. A straight forward extension would be to oscillate the secondary laser in time. This can be used to measure the dynamical response of this system to the local dipole field, an interesting theoretical problem, which we leave for future work.

The second part of our analysis addressed the effect of coupling between parallel one dimensional chains, which is inherent to realization with an optical lattice. As a simple model for the coupled chains we analyzed the case of two coupled chains, using a bosonization approach in section II D and numerical simulations with DMRG in sections III C and III D. The natural couplings to consider are inter chain repulsion due to the dipolar moment of the atoms or molecules and the inter-chain tunneling. The interaction coupling turns out to be essentially trivial and does not change the structure of the phase diagram. The inter-chain tunnel coupling, on the other hand, has a dramatic effect. Like the inversion symmetry breaking perturbation discussed above, this perturbation eliminates the distinction between the MI and HI phases. However, instead of gapping out the critical point, it expands it into a phase. More precisely, a weak inter chain tunneling gives rise to an intermediate superfluid phase, whose domain grows quickly with the coupling strength. The transition from the superfluid to either the Haldane or Mott insulator is Kosterlitz-Thouless like and occurs at the universal value of the decay exponent of the single particle density matrix.

The evolution of the phase diagram with increasing inter-chain coupling for the case of many coupled chains and more general interactions deserves further theoretical study. This may provide a controlled route for investigating the crossover from one to two dimensions. Of particular interest is the question of possible generalizations of the string orders to the case of two (or at least quasi one) dimensional systems.

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APPENDIX A: STRING CORRELATIONS AT WEAK INTER-CHAIN COUPLING

In this appendix we derive the effect of weak inter-chain coupling terms on the long range string correlations in the HI phase. For simplicity we will study this within the effective spin-1 model that results from restriction to three occupation states $n = 0, 1, 2$ on each site[21,22]:

$$\begin{aligned} H_{eff} &= -\frac{t\bar{n}}{2}\sum_{\langle ij\rangle}\left(S_i^+S_j^- + H.c.\right) + \frac{U}{2}\sum_i (S_i^z)^2 \\ &+V\sum_{\langle ij\rangle} S_i^z S_j^z - \mu\sum_i S_i^z \\ &-t\bar{n}\xi\sum_{\langle ij\rangle}\left(S_i^-(S_i^z+S_j^z)S_j^+ + H.c.\right) \\ &-\frac{t\bar{n}\xi^2}{2}\left(S_i^zS_i^+S_j^-S_j^z + S_i^+S_i^zS_j^zS_j^-\right) \end{aligned} \quad \text{(A1)}$$

where $\xi = \sqrt{2}-1$ for a system single average occupation. Here we shall set $\xi = 0$, essentially neglecting terms that break the particle hole symmetry. Possible effects of these terms, which deserve further study, will be briefly discussed at the end of this section.

Next we follow Kennedy and Tasaki and define a non local unitary transformation of the spins on all lattice sites

$$U = \prod_{jk|j<k} e^{i\pi S_j^z S_k^x} \quad \text{(A2)}$$

The Hamiltonian gains an unusual, but nonetheless local form, in terms of the transformed spin variables:

$$\begin{aligned} \tilde{H} &= -J\sum_j \tilde{S}_j^x\tilde{S}_{j+1}^x - \tilde{S}_j^y\exp(i\pi\tilde{S}_j^z + i\pi\tilde{S}_{j+1}^x)\tilde{S}_{j+1}^y \\ &-V\sum_j \tilde{S}_j^z\tilde{S}_{j+1}^z + \frac{U}{2}\sum_j(\tilde{S}_j^z)^2. \end{aligned} \quad \text{(A3)}$$

$\tilde{H}$ has an explicit $Z_2\times Z_2$ symmetry, generated by π rotations of the transformed spins around the main axes. Furthermore the non local string correlations of the original spins map to standard two point correlations of the transformed spins. In the Haldane phase the $Z_2\times Z_2$ symmetry is broken, and the transformed spin operators gain a finite expectation value.

We can therefore treat the Haldane phase of $\tilde{H}$ with a mean field approximation[13], in which the four degenerate broken symmetry ground states are given by the product wavefunctions:

$$|\,\Psi_{\zeta,\eta}\,\rangle = \prod_i\left(\cos\theta\,|\,0\,\rangle_i + \zeta\sin\theta\,|\,\eta 1\,\rangle_i\right). \quad \text{(A4)}$$

The labels $\zeta,\eta = \pm 1$ correspond to the signs of the two Z_2 order parameters $\langle\tilde{S}_i^x\rangle$, and $\langle\tilde{S}_i^z\rangle$. The elementary excitations in this phase are domain walls separating any two of the degenerate ground states. Interestingly such domain walls are generated by acting on a ground state

with the original spin operators:

$$\begin{aligned} S_i^x &= \tilde{S}_i^x \exp(i\pi \sum_{j>i} \tilde{S}_j^x) \\ S_i^y &= \exp(i\pi \sum_{j<i} \tilde{S}_j^z) \tilde{S}_i^y \exp(i\pi \sum_{j>i} \tilde{S}_j^x) \\ S_i^z &= \exp(i\pi \sum_{j<i} \tilde{S}_j^z) \tilde{S}_i^z \end{aligned} \tag{A5}$$

Thus S_i^x creates a kink in η ($\langle \tilde{S}_i^z \rangle$), S_i^z creates a kink in ζ ($\langle \tilde{S}_i^x \rangle$), and S_i^y creates kinks in both order parameters. As in any Ising system, proliferation of a finite density of domain walls leads to destruction of the order. This is the mechanism by which inter-chain coupling destroys the long range string correlations.

Consider first the perturbative effect of the inter-chain interaction $H_{V_\perp} = V_\perp \sum_i S_{1i}^z S_{2i}^z$. The correction to the ground state to first order in $V_\perp/\Delta$ consists of a single domain wall in the $\langle \tilde{S}_i^x \rangle$ order parameter in each chain. If we consider higher order terms, the weight of a configuration with n domain walls per chain scales as $(V_\perp/\Delta)^n$ and the density of domain walls of $\langle \tilde{S}_i^x \rangle$ in the ground state is $\propto V_\perp/\Delta$. Therefore we expect the S^x string correlations to decay exponentially over a correlation length $\xi_x \sim \Delta/V_\perp$. On the other hand the S^z string order is left unmodified by this perturbation.

We can apply a similar argument to the inter-chain tunneling term $H_{t_\perp} = -t_\perp \sum_i (S_i^x S_j^x + S_i^y S_j^y)$.

APPENDIX B: ALTERNATIVE BOSONIZATION SCHEME

In section II we derived the continuum field theory in a rather indirect way. In the first step the EBHM (1) was mapped to the effective spin-1 model A1. We then followed the procedure developed in Refs. [11,12] for such spin systems which involves: (i) splitting a spin-1 chain into two effective spin-1/2 chains; (ii) fermionizing the parallel spin-1/2 chains with a Jordan-Wigner transformation; (iii) Bosonizing the fermions.

There is a standard procedure to "bosonize" a bosonic Hamiltonian[17,32], and it is tempting to ask why not to use this more direct approach to derive the field theory which describes the transitions between the MI, HI and DW phases. This turns out to be not so trivial.

The standard scheme is based on expansion of the fluctuations of the discrete particle density to slow modes describing small deviations from the fundamental period set by the average density and its harmonics $k_n = 2\pi n \rho_0$:

$$\rho(x) \to \left(\rho_0 - \frac{1}{\pi} \partial_x \phi(x) \right) \sum_{n \in \mathbb{Z}} e^{i(k_n x_i - 2n\phi(x_i))} \tag{B1}$$

Thus, slow variations around the fourier component $k = nk_0$ of the density are given by the field $\cos(2n\phi(x))$. A finite expectation value for this field implies a static density wave, with the periodicity $\lambda_n = 2\pi/k_n = 1/(n\rho_0)$ in the ground state. Clearly the period $2a$ density generated at unity filling by a strong nearest-neighbor interaction V is not captured in this expansion (here $\rho_0 = 1/a$, with a the lattice spacing). It is therefore not surprising that the Haldane insulator, which involves fluctuations at the same length scale and is in some sense a precursor of the DW phase, cannot be described in this approach either.

We now propose a modified bosonization procedure that will enable us to derive the low energy field theory (6). The key idea is to split a bosonic chain into two auxiliary chains without changing the total number of bosons. In other words, a single chain with one boson per site maps to a ladder with one boson per rung, or one boson in every two sites in each of the auxiliary chains. Next each of the half filled chains is bosonized separately in the standard way

$$\begin{aligned} b_{\alpha i} &= e^{i\theta_\alpha(x_i)} \left(\frac{1}{2a} - \frac{1}{\pi} \partial_x \phi_\alpha(x_i) \right)^{1/2} \\ &\quad \times \sum_{m \in \mathbb{Z}} e^{i(\frac{m\pi}{a} x_i - 2m\phi_\alpha(x_i))} \\ \delta\rho_\alpha(x_i) &= \left(\frac{1}{2a} - \frac{1}{\pi} \partial_x \phi_\alpha(x_i) \right) \sum_{m \in \mathbb{Z}} e^{i(\frac{m\pi}{a} x_i - 2m\phi_\alpha(x_i))} \end{aligned} \tag{B2}$$

where $\alpha = 1, 2$ is the auxiliary chain index. Note that the correct wave-vector to describe the DW has emerged from the inverse density of each of the split chains. We anticipate that the density wave of the physical chain will appear as in-phase locking of density waves in the two auxiliary half filled chains.

We now map the EBHM (1) to a closely related model on the auxiliary ladder by taking $b_i \to (b_{1i} + b_{2i})/\sqrt{2}$ and $n_i \to n_{1i} + n_{2i}$. Choosing a slightly different extension of the BHM to the auxiliary ladder system should not change the essential structure of the phase diagram. The naive continuum limit of this model can now be taken by using the identities (B2). For the on-site interaction term we obtain:

$$\frac{U}{2} \sum_i (n_{1,i} + n_{2,i} - 1)^2 \approx \frac{Ua}{2} \int dx \Big[\frac{1}{\pi^2} (\partial\phi_+)^2 - \frac{1}{a^2} \cos(2\phi_+) \cos(2\phi_+) + \frac{1}{a^2} \big(\cos(2\phi_+) + \cos(2\phi_-) \big) \Big] \tag{B3}$$

where $\phi_\pm \equiv \phi_1 \pm \phi_2$, and we have kept only the most relevant terms. Similarly the nearest neighbor interaction term

leads to

$$\frac{V}{2}\sum_i (n_{1,i}+n_{2,i}-1)(n_{1,i}+n_{2,i}-1) \approx Va\int dx\Big[\frac{1}{\pi^2}(\partial\phi_+)^2-\frac{1}{a^2}\cos(2\phi_+)\cos(2\phi_-)-\frac{1}{a^2}\Big(\cos(2\phi_+)+\cos(2\phi_-)\Big)\Big] \quad \text{(B4)}$$

Finally the hopping term translates to

$$\begin{aligned}\frac{t}{2}\sum_i\sum_{\alpha,\beta=1}^{2} b^\dagger_{\alpha i}b_{\beta i+1}+H.c. \;\approx\; \frac{t}{2}\int dx\Big[&\big(a(\partial\theta_+)^2+a(\partial\theta_-)^2\big)\left(1+\cos(2\theta_-)\right)-\frac{4}{a}\cos(2\phi_+)\cos(2\phi_-)(1+2\cos(2\theta_-))\\ &+\left(-\frac{a}{4\pi^2}(\partial\phi_-)^2+\frac{4}{a}\cos(2\phi_+)+\frac{4}{a}\cos(2\phi_-)-\frac{2}{a}\right)\cos(2\theta_-)\Big]. \end{aligned} \quad \text{(B5)}$$

Here $\theta_\pm \equiv (\theta_1 \pm \theta_2)/2$. Note that we have essentially the same degrees of freedom here as in section II A. In the MI and HI phases the operator $\cos(2\theta_-)$ is relevant and we can safely replace it with its expectation value C_- which is of order 1. In this case the above expressions simplify and give precisely the field theory (6) with the parameters:

$$\begin{aligned} K_+ &= \pi\sqrt{\frac{\frac{t}{2}(1+C_-)}{\frac{U}{2}+V}}, \quad K_- = 2\pi\sqrt{\frac{1+C_-}{C_-}} \\ g_1 &= g_2 = \pi^2 a\left(\frac{U}{2}-V-2tC_-\right), \quad g_3 = -\pi a t \\ g_4 &= -\pi^2 a\left[\frac{U}{2}+V+2t\left(1+2C_-\right)\right] \end{aligned} \quad \text{(B6)}$$

Note that the bare value of the Luttinger parameter K_- of the antisymmetric fields is large ($K_- > 2\pi$), consistent with taking C_- of order 1.

Before closing this appendix let us make a few remarks concerning the new scheme. First note that the bare value of the Luttinger parameter K_+ implies a reasonable estimate for the phase boundary between the superfluid and insulating phases. The system should be superfluid when the renormalized Luttinger parameter $\tilde{K}_+$ exceeds 2. Estimating this criterion with the bare value given above we get the approximate criterion $(U+2V)/t < \pi^2/4$. By contrast the spin-1 mapping predicted that there is no superfluid phase in the region $U > 0$ and $V > 0$. Indeed we do not expect the spin-1 mapping, which involves truncation to 3 occupation states, to hold when the on-site repulsion is not sufficiently strong. Thus the new scheme improves on the the spin one mapping in that it gives reasonable predictions for the phase diagram already at the level of the naive continuum limit.

Another notable difference between the field theory of section II A and the new scheme is a π shift in the definition of the field ϕ_+. Hence in the bosonic scheme $\phi_+ \approx \pi$ corresponds to the MI phase whereas $\phi_+ \approx 0$ to the HI. This is consistent with the physical interpretation of the variable ϕ_+ in the new scheme. Consider first the DW phase, which corresponds to a phase locked density wave on the two auxiliary chains. For this we need ϕ_1=$\phi_2 \approx 0$. Since ϕ_+ is not critical at the transition from DW to HI we expect $\phi_+ \approx 0$ also in the HI phase.

APPENDIX C: THE STRING AND PARITY ORDER PARAMETERS

The HI and MI phases do not support long range order in any local order parameter. Instead, they are characterized by the non-local string and parity order parameters (Eqs. (15,14), respectively). In order to obtain the bosonized expressions for these order parameters in the effective field theory, we need to find their continuum limit. Here we propose a continuum form of these operators using general considerations based on the asymptotic "particle-hole" symmetry of the model at low energy. More microscopic derivations can be found in Refs. [26,29]

In the following argument, we will assume that it is legitimate to truncate the Hilbert space to the three lowest occupation numbers ($\delta n_j = 0, \pm 1$). δn can then be represented by a pseudospin-1 degree of freedom, defined by $S^z_j = \delta n_j$. The model (1) is then replaced by the effective spin-1 model of Eq. (4), which leads to the same low energy effective theory (7,8). We have neglected terms that break the symmetry between $S^z_j = -1$ and $S^z_j = 1$ ("particle-hole" symmetry). These terms appear in Eq. (A1). They are irrelevant at low energies, so neglecting them should not change the long-distance behavior.

Next, we need to find the continuum limit of the operators $\hat{\mathcal{O}}_P(j)$ and $\hat{\mathcal{O}}_S(j)$. Taking the naive continuum limit of $\hat{\mathcal{O}}_P(j)$, we get $\hat{\mathcal{O}}_P \sim e^{i\phi_+}$ (since $\sum_{j<i} S^z_j \to \int^x dx' S^z(x') = \frac{1}{\pi}\phi_+(x)$, assuming that $\phi_+(-\infty) = 0$)[28,29,30]. To get a hermitian operator, $e^{i\phi_+}$ has to be symmetrized. To find the correct symmetrization, we note that $\hat{\mathcal{O}}_P(j)$ should be symmetric under a "particle-hole" transformation (which correspond under bosonization to $\phi_+ \to -\phi_+$). Therefore, $\hat{\mathcal{O}}_P$ should have the form

$$\hat{\mathcal{O}}_P \sim A_P \cos(\phi_+) + ... \quad \text{(C1)}$$

where A_P is a non-universal constant, and we have truncated additional sub-leading operators of this sum. $\hat{\mathcal{O}}_S(j)$ also contains the same $e^{i\phi_+}$ factor, but it should

be anti-symmetric under a particle-hole transformation, which suggests the general form

$$\hat{\mathcal{O}}_S = A_S \sin(\phi_+) + B_S \partial_x \phi_+ \cos(\phi_+) + ... \qquad \text{(C2)}$$

The second contribution in Eq. (C2) is expected from naively bosonizing Eq. (15) and taking Eq. (C1) into account. However, a more careful treatment of the operator product expansion for this expression [26,29] shows that the first term is also present. The $\sin(\phi_+)$ term is the most relevant one. From Eqs. (C1,C2) we see that in the MI phase, where ϕ_+ is pinned around 0, we expect that $\langle \hat{\mathcal{O}}_P \rangle \neq 0$, $\langle \hat{\mathcal{O}}_S \rangle = 0$, while in the HI ϕ_+ is pinned around $\pm\pi/2$, therefore $\langle \hat{\mathcal{O}}_P \rangle = 0$, $\langle \hat{\mathcal{O}}_S \rangle \neq 0$. In order to test the validity of these results for the EBHM [Eq. (1)], where particle-hole breaking terms exist, we evaluate the string and parity correlation functions in (12,13) numerically across the MI→HI transition. The results, summarized in Figs. 4,5, are consistent with Eqs. (C1,C2).

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